



# Setting Expectations for Performance Portability between Companion Accelerator and Manycore Systems

John M Levesque  
Director  
Cray's Supercomputing Center of Excellence  
CTO Office

# Outline

- **Look at recent research in Europe**
  - Tuning the implementation of the radiation scheme ACRANEB2
    - Jacob W. Poulsen and Per Berg *IT department, DMI*
    - *Most of the slides I will be using were generated by Jacob and Per*
- **Conclusions**

# Real World Climate Model Issue



- **ACRANEB2 is the radiation scheme used in the IFS code**
  - Currently the radiation scheme is used intermittently, researchers would like to use it every time step
  - Highly compute intensive unlike other parts of climate modeling which tend to be memory bandwidth limited
- **Radiation scheme ported to KNL and Nvidia**
  - Then code was optimized for KNL using OpenMP (SPMD)
  - Then code was optimized further for P100 using OpenACC
- **Performance tests performed on KNL, P100 and Broadwell**

## Intermezzo: Musings on performance

- ▼ Think of a programming language and a parallel programming model as a short-hand notation for generating specific code for a given target.
- ▼ **Do not buy the appealing idea** that you can construct efficient programs solely by using the abstractions of programming languages and parallel programming models.
- ▼ Sorry to say but you have to understand how the target architecture works if performance truly matters to you and you might instead think of the process of writing code as a process where you try to hint the compiler etc. in the right direction towards a given target architecture.
- ▼ ...and again if performance matters to you:
- ▼ Think of a programming language and a parallel programming model as a short-hand notation for generating specific code for a given target.

## Intermezzo: Musings on performance

- Abstractions are very appealing from a computer scientific point of view but don't get fooled. Abstractions are never free, 2D arrays can be too much of an abstraction if performance is key.

```
!- 2D abstractions too complicated -----  
1 do k=2, kmax  
2   k1 = k+off1  
3   k2 = k+off2  
4   t(1:nc,k) = t(1:nc,k) + A(k)*(B(1:nc,k1)-B(1:nc,k2))  
5 enddo
```

- With dynamic **nc** the compiler vectorizes **nc**-loop:  
(4): (col. 7) remark: LOOP WAS VECTORIZED
- With static **nc**, the compiler vectorizes the **k**-loop:  
(1): (col 7) remark: LOOP WAS VECTORIZED
- Alas, assembler inspection revealed that gather operations were generated and runtime experiences confirm this.
- ...

## Intermezzo: Musings on performance

- ▼ Programming languages and parallel programming models have several options when it comes to architectural features

(Brent Leback et al, cug2013):

- ▼ Hide
  - ▼ Virtualize
  - ▼ Expose
- 
- ▼ OpenMP has a **good** reputation productivitywise – why ?
  - ▼ OpenMP has a **bad** reputation performancewise – why ?
  - ▼ OpenMP is a highly abstract model so very **easy to use and misuse**
- 
- ▼ MPI has a **bad** reputation productivitywise – why ?
  - ▼ MPI has a **good** reputation performancewise – why ?
  - ▼ MPI exposes the separate nodes, the distributed memory and all “network” transfers explicitly **so the programmer will have to consider how to deal with these details** while implementing the program

# Refactoring of legacy code



1. Establish a solid **reference** (test case and source code) that reproduces the necessary results.
2. Establish **build** and **run env.** to ease repetition and reproducibility.
3. Ensure proper **threading**, i.e. SPMD approach
  - requires transition to Fortran90 assumed-shape and trimming stack memory usage
  - contiguous data
4. Strive towards a **minimal implementation**, including:
  - Reduce memory overhead
  - Reduce stack pressure: local tmp 2D/3D vars into 1D/2D vars or even scalars
  - Largest stack arrays moved to the heap; proper NUMA initialization of heap arrays
  - Collapsing loops over the outermost index
  - Symbolic algebraic reduction using pen&paper
  - Assuring no side effects in local functions (**pure** in Fortran)
  - Declare constants as constants (**parameter** in Fortran), not as variables
  - Push all branching out of the loops
5. Continued refactoring is to shuffle computations around to **maximize parallel exposure** (playing with data structures and loops)
  - Identify computational patterns with (e.g. reduction and prefix-sum) and without (SIMD-suitable loops) dependencies
  - Re-organize heavy loops to constant trip-count
  - ...

# Tuning for short latency capacity per compute unit



**Some P100 specs:** 56 SM (streaming multiprocessor) per GPU

32 DP cuda cores per SM

Scheduling unit is a **warp** [device limit: max 64 warps per SM]

Always 32 **threads** per warp [i.e. max 2048 active threads per SM]

**Thread block** [device limit: max 32 blocks per SM]:

Block size is #thread [device limit: max 1024 threads per block]

Default block has **128** threads and 4 warps

Blocks are "tunable" wrt #warps and #threads per block

[device limits: max 1024 threads and max 32 warps per block]

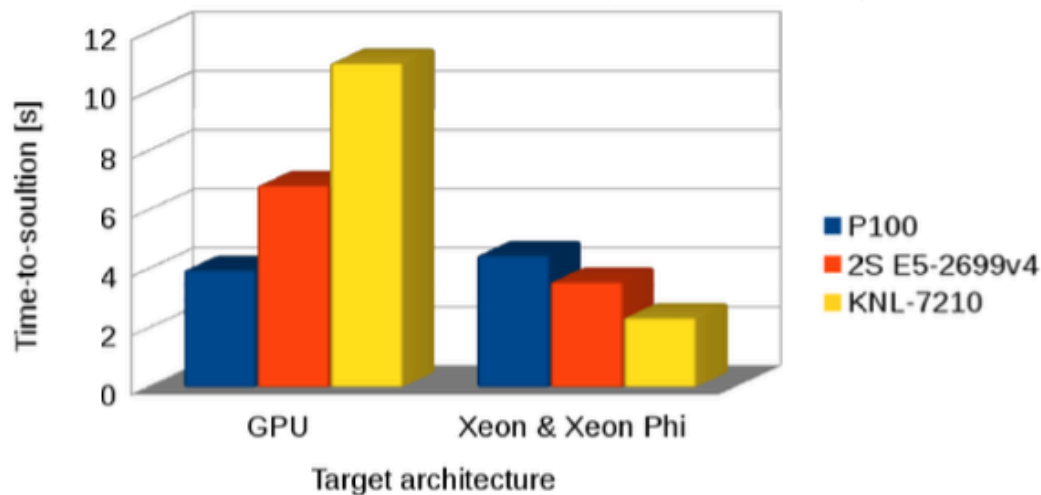
**Registers:** 256KB register file per SM

[device limits: **max 65536 32bit regs per SM,**  
max 65536 registers per block,  
max 255 registers per thread]

So, tuning for short latency capacity on P100 is about **keeping #registers per thread low**

Measure is **occupancy:** **#active threads in percent of device limit**

# Portable vs competitive performance

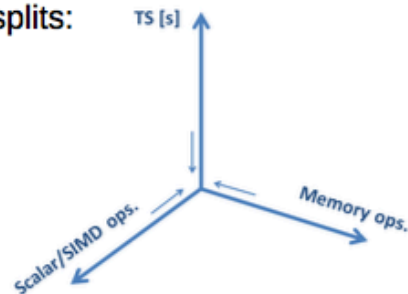


Note 1: **X** and **G codes** are essentially the same, except for the splits:

One must be able to hide the memory latencies resulting from extra memory transfers required to bind the smaller parts.

Note 2: **X** and **G codes** still has prefix-sum loops:

High scalar/SIMD might hurt performance.



# Effect of refactoring

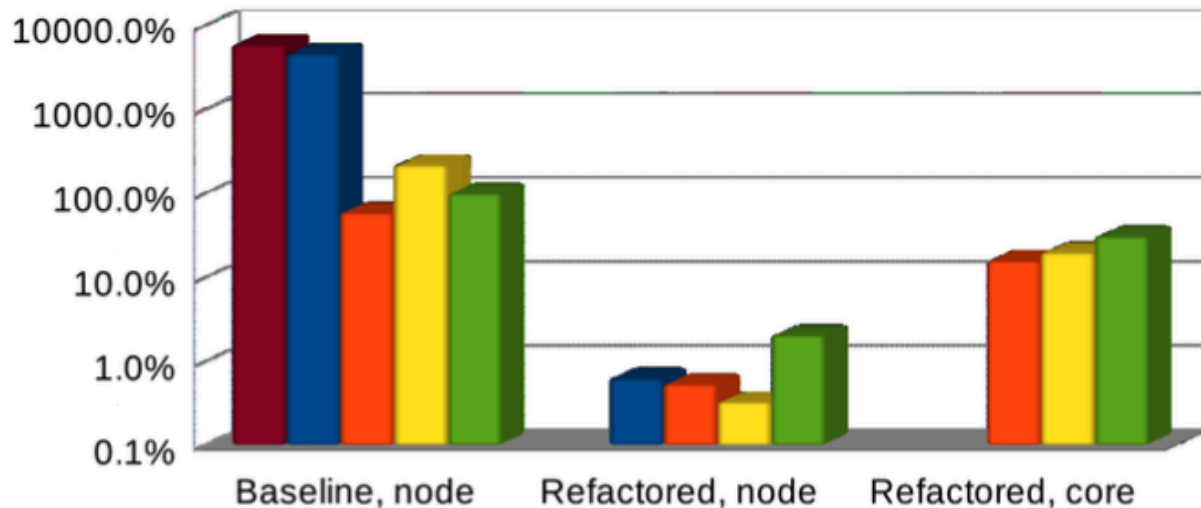


Refactoring is increasingly more important the newer the hardware  
– legacy codes might even run slower on more modern HW

Refactoring is even more important for the high throughput architectures

Timings of TRANST in full ACRANEB2 relative to baseline code on SNB:

■ K20x ■ P100 ■ 2S E5-2699v4 ■ KNL-7210 ■ 2S E5-2680v1



# Hardware Counters for both X and G on Broadwell



TRANST3 Running on Broadwell	KNL Version - X      13.7%peak(DP)	GPU Version - G      3.1%peak(DP)
HW FP Ops    Uptime	2,704.935M /sec      20,260,160,826	497.003M/sec      13,489,461,656
Total SP Ops	13.356M/ sec      100,035,301	6.621M/sec      179,715,564
Total-DP-ops	2,691.579M /sec      20,160,125,525	490.381M/sec      13,309,746,092
Computational-intensity	1.1 ops/ cycle      3.81 ops/ref	0.25 ops/cycle      1.52 ops/ref
MFLOPS(aggregate)	2,704.94M/ sec      3088.61	497.00M/sec
TLButilization	refs/miss      6.03 avg uses	540.74 refs/miss      1.06 avg uses
D1cachehit,missratios	93.6% hits      6.4% misses	95.5% hits      4.5% misses
D1cacheutilization	15.71refs/ miss      1.96 avg hits	22.38refs/miss      2.80 avg hits
D2cachehit,missratio	59.6% hits      40.4% misses	79.8% hits      20.2% misses
D1+D2cachehit,miss	97.4% hits      2.6% misses	99.1% hits      .1% misses
D1+D2 cacheutilization	38.94 refs/ miss      4.87 avg hits	110.78 refs/miss      13.85 avg hits
D2toD1bandwidth	1,546.057Mi B/sec      12,142,593,984 bytes	440.315MiB/sec      12,531,398,336 bytes

# Hardware Counters for both X and G on Broadwell



TRANST3 Running on Broadwell	KNL Version - X	13.7%peak(DP)	GPU Version - G	3.1%peak(DP)
HW FP Ops Usertime	2,704.935M/sec	20,260,160,826	497.003M/sec	13,489,461,656
Total SP Ops	13.356M/sec	100,035,301	6.621M/sec	179,715,564
Total-DP-ops	2,691.579M/sec	20,160,125,525	490.381M/sec	13,309,746,092
Computational-intensity	1.1 ops/cycle	3.81 ops/ref	0.25 ops/cycle	1.52 ops/ref
MFLOPS(aggregate)	2,704.94M/sec		497.00M/sec	
			540.74 refs/	
TLButilization	3088.61 refs/miss	6.03 avg uses	miss	1.06 avg uses
D1cachehit,missratios	93.6% hits	6.4% misses	95.5% hits	4.5% misses
D1cacheutilization	15.71refs/miss	1.96 avg hits	22.38refs/miss	2.80 avg hits
D2cachehit,missratio	59.6% hits	40.4% misses	79.8% hits	20.2% misses
D1+D2cachehit,miss	97.4% hits	2.6% misses	99.1% hits	.1% misses
			110.78 refs/	
D1+D2 cacheutilization	38.94 refs/miss	4.87 avg hits	miss	13.85 avg hits
		12,142,593,984		12,531,398,336
D2toD1bandwidth	1,546.057MiB/sec	bytes	440.315MiB/sec	bytes

# Results of X and G code running on Broadwell – 8.2

## Seconds with memory analysis



Samp%	Samp	Imb.	Imb.	MEM_LOAD_UOPS_RETIRED	RESOURCE_STALLS	Group
		Samp	Samp%	:HIT_LFB:precise=2	:ALL	Function=[MAX10]
						Source
						Line
100.0%	94.0	--	--	37,600,846	18,471,464,610	Total
-----						
	70.2%	66.0	--	--	26,400,588	13,003,862,681   USER
-----						
	70.2%	66.0	--	--	26,400,588	13,003,862,681   acraneb_transt3\$acraneb3__clone_31615_1501851751_2_
3						acraneb2.f90
4						line.130

X

Samp%	Samp	Imb.	Imb.	MEM_LOAD_UOPS_RETIRED	RESOURCE_STALLS	Group
		Samp	Samp%	:HIT_LFB:precise=2	:ALL	Function=[MAX10]
						Source
						Line
100.0%	44.0	--	--	17,600,396	40,138,321,643	Total
-----						
	70.5%	31.0	--	--	12,400,279	30,022,721,717   USER
-----						
	70.5%	31.0	--	--	12,400,279	30,022,721,717   acraneb_transt3\$acraneb3_
3						acraneb3.F90
=====						

G

# Results of X and G code running on KNL with memory analysis



X

Samp%	Samp	Imb. Samp	Imb. Samp%	NO_ALLOC_CYCLES :ALL	MEM_UOPS_RETIRED :L2_MISS_LOADS :precise=2	Group Function=[MAX10] Source Line
50.0%	2.0	--	--	4,050,957,765	80,025	USER
50.0%	2.0	--	--	4,050,957,765	80,025	acraneb_transt3\$acraneb3__clone_3707_1501852873_
3						acraneb2.f90
4						line.130

G

Samp%	Samp	Imb. Samp	Imb. Samp%	NO_ALLOC_CYCLES :ALL	MEM_UOPS_RETIRED :L2_MISS_LOADS :precise=2	Group Function=[MAX10] Source Line
100.0%	22.0	--	--	95,250,152,816	880,198	Total
90.9%	20.0	--	--	90,890,511,782	800,181	USER
86.4%	19.0	--	--	90,799,881,468	760,155	acraneb_transt3\$acraneb3_
3						acraneb3.F90

# Code Optimized for KNL

```
100.0% | 1,271.608331 |      -- | Total
|-----|
| 100.0% | 1,271.602597 |      1.0 | foo_
| 100.0% | 1,271.602595 |      1.0 | main_
3 99.9% | 1,270.601680 |      2.0 |  radia_dwarf$radia_m_
4 99.9% | 1,270.463249 |      1.0 |  acraneb2$acraneb2_m_
5 99.9% | 1,270.463240 |      2.0 |  acraneb_transt3$acraneb3_
6 99.9% | 1,270.463238 |      -- |  acraneb_transt3$acraneb3_.LOOP.1.li.238 (160,000)
7 99.9% | 1,270.176018 |      -- |  acraneb_transt3$acraneb3_.LOOP.3.li.305 (40)
8 99.2% | 1,260.805241 |      -- |  acraneb_transt3$acraneb3_.LOOP.6.li.485 (81)
|||||||-----|
9||||||| 25.4% | 323.354494 | 518,400,000.0 | zcdel0$acraneb3_
9||||||| 22.7% | 288.227424 | 518,400,000.0 | ztdel1$acraneb3_
9||||||| 15.0% | 190.522204 | 518,400,000.0 | zcdelta1$acraneb3_
9||||||| 14.4% | 182.970033 | 518,400,000.0 | ztdelta1$acraneb3_
9||||||| 11.1% | 141.669216 | 518,400,000.0 | zcdelta2$acraneb3_
9||||||| 10.5% | 134.061872 | 518,400,000.0 | ztdelta2$acraneb3_
|=====|
```

Table 1: Function Calltree View

Time%	Time	Calls	Calltree
100.0%	1,177.513999	--	Total
-----			
100.0%	1,177.508949	1.0	foo_
100.0%	1,177.508947	1.0	main_
3 99.8%	1,174.984080	2.0	radia_dwarf\$radia_m_
4 99.8%	1,174.845679	1.0	acraneb2\$acraneb2_m_
5 99.8%	1,174.845669	2.0	acraneb_transt3\$acraneb3_
6 99.8%	1,174.845665	--	acraneb_transt3\$acraneb3_.LOOP.0001.li.210 (2)
-----			
7	27.1%	319.289605	--   acraneb_transt3\$acraneb3_.LOOP.0014.li.469 (80,000)
8	27.1%	319.157763	--   acraneb_transt3\$acraneb3_.LOOP.0016.li.502 (40)
9	26.4%	311.138577	--   acraneb_transt3\$acraneb3_.LOOP.0019.li.567 (81)
10	26.4%	311.138577	518,400,000.0   zcdel0\$acraneb3_
7	24.8%	291.704217	--   acraneb_transt3\$acraneb3_.LOOP.0026.li.657 (80,000)
8	24.8%	291.496028	--   acraneb_transt3\$acraneb3_.LOOP.0028.li.701 (40)
9	24.0%	283.149544	--   acraneb_transt3\$acraneb3_.LOOP.0031.li.803 (81)
-----			
10	13.5%	159.425912	518,400,000.0   ztdelta1\$acraneb3_
10	10.5%	123.723632	518,400,000.0   ztdelta2\$acraneb3_
=====			
7	24.0%	282.573841	--   acraneb_transt3\$acraneb3_.LOOP.0032.li.832 (80,000)
8	24.0%	282.452776	--   acraneb_transt3\$acraneb3_.LOOP.0034.li.865 (40)
9	23.4%	274.949679	--   acraneb_transt3\$acraneb3_.LOOP.0037.li.934 (81)
10	23.4%	274.949679	518,400,000.0   ztdel1\$acraneb3_
7	13.5%	158.979422	--   acraneb_transt3\$acraneb3_.LOOP.0002.li.218 (80,000)
8	13.5%	158.788738	--   acraneb_transt3\$acraneb3_.LOOP.0004.li.254 (40)
9	12.9%	151.482292	--   acraneb_transt3\$acraneb3_.LOOP.0007.li.323 (81)
10	12.9%	151.482292	518,400,000.0   zcdelta1\$acraneb3_
7	10.4%	122.140792	--   acraneb_transt3\$acraneb3_.LOOP.0008.li.347 (80,000)
8	10.4%	121.957475	--   acraneb_transt3\$acraneb3_.LOOP.0010.li.380 (40)
9	9.8%	114.865167	--   acraneb_transt3\$acraneb3_.LOOP.0013.li.445 (81)
10	9.8%	114.865167	518,400,000.0   zcdelta2\$acraneb3_
=====			


# Code Optimized for GPU



## Further tuning – 2



Sketch of latest GPU target code: nproma & 12-way split, GN code

C1.1  
C1.2  
C2.1  
C2.2  
C3   
Crest  
T1.1  
T1.2  
T2.1  
T2.2  
T3  
Trest

C3 chunk as an example:

!\$acc parallel

Jlon-loop, **stride nproma**:

Jlev-loop:

i=1,nproma:

Preparation: 8 (5 RO, 3 WO)

Jlev1-loop:

Jlev2-loop:

i=1,nproma:

Prefix-sum: 12 (3+2+1 RO, 6 WO)

Jlev2-loop:

i=1,nproma:

Fat loop: 8+1 (6+1 RO, 1 WR)

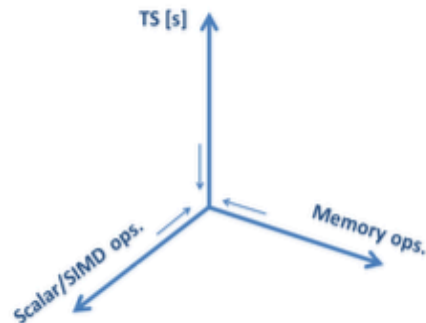
## Further tuning – 2



**GN code:** scalar/SIMD ratio decreases, so does occupancy:  
Result is that T2S decreases by 1.7x:

**25 - 43.75%**  
**T2S = 2.32 s**

Part	regs/thread	theoretical occupancy [%]
C1.1	96	31.25
C1.2	72	43.75
C2.1	94	31.25
C2.2	72	43.75
C3	118	25
Crest	94	31.25
T1.1	96	31.25
T1.2	72	43.75
T2.1	94	31.25
T2.2	72	43.75
T3	112	25
Trest	80	37.50



# Loop Table for NPROMA =32 run



Table 2: Inclusive and Exclusive Time in Loops (from -hprofile\_generate)

Loop Incl Time%	Loop Incl Time	Time (Loop Adj.)	Loop Hit	Loop Trips Avg	Loop Trips Min	Loop Trips Max	Function=/.LOOP[.]
131.8%	2,090.202939	0.000008	1	2.0	2	2	acraneb_transt3\$acraneb3_.LOOP.0001.li.179
23.8%	378.109848	0.003810	2	625.0	625	625	acraneb_transt3\$acraneb3_.LOOP.0050.li.607
23.8%	378.047825	0.302535	1,250	40.0	40	40	acraneb_transt3\$acraneb3_.LOOP.0053.li.633
23.7%	375.755567	0.038828	50,000	81.0	81	81	acraneb_transt3\$acraneb3_.LOOP.0060.li.713
23.7%	375.716739	44.147064	4,050,000	128.0	128	128	acraneb_transt3\$acraneb3_.LOOP.0061.li.719
23.4%	370.373284	0.003828	2	625.0	625	625	acraneb_transt3\$acraneb3_.LOOP.0121.li.1223
23.4%	370.312884	0.308230	1,250	40.0	40	40	acraneb_transt3\$acraneb3_.LOOP.0124.li.1249
23.2%	368.024567	0.039692	50,000	81.0	81	81	acraneb_transt3\$acraneb3_.LOOP.0131.li.1330
23.2%	367.984875	44.315884	4,050,000	128.0	128	128	acraneb_transt3\$acraneb3_.LOOP.0132.li.1336
15.2%	240.320211	0.014168	2	2,500.0	2,500	2,500	acraneb_transt3\$acraneb3_.LOOP.0073.li.807
15.1%	240.165708	1.060907	5,000	40.0	40	40	acraneb_transt3\$acraneb3_.LOOP.0076.li.832
15.0%	238.259467	0.014077	2	2,500.0	2,500	2,500	acraneb_transt3\$acraneb3_.LOOP.0002.li.188
15.0%	238.104327	1.013176	5,000	40.0	40	40	acraneb_transt3\$acraneb3_.LOOP.0005.li.213
14.9%	235.604348	0.131438	200,000	81.0	81	81	acraneb_transt3\$acraneb3_.LOOP.0083.li.896
14.8%	235.472911	48.302278	16,200,000	32.0	32	32	acraneb_transt3\$acraneb3_.LOOP.0084.li.902
14.7%	233.629111	0.134209	200,000	81.0	81	81	acraneb_transt3\$acraneb3_.LOOP.0012.li.278
14.7%	233.494902	46.806381	16,200,000	32.0	32	32	acraneb_transt3\$acraneb3_.LOOP.0013.li.283
13.0%	206.404953	0.013350	2	2,500.0	2,500	2,500	acraneb_transt3\$acraneb3_.LOOP.0097.li.1024
13.0%	206.301616	1.019964	5,000	40.0	40	40	acraneb_transt3\$acraneb3_.LOOP.0100.li.1047
12.8%	202.361857	0.145688	200,000	81.0	81	81	acraneb_transt3\$acraneb3_.LOOP.0107.li.1102
12.8%	202.216170	50.037572	16,200,000	32.0	32	32	acraneb_transt3\$acraneb3_.LOOP.0108.li.1107
11.5%	182.050951	0.013106	2	2,500.0	2,500	2,500	acraneb_transt3\$acraneb3_.LOOP.0026.li.402
11.5%	181.948361	1.003706	5,000	40.0	40	40	acraneb_transt3\$acraneb3_.LOOP.0029.li.424
11.2%	178.034804	0.131957	200,000	81.0	81	81	acraneb_transt3\$acraneb3_.LOOP.0036.li.481
11.2%	177.902847	48.839249	16,200,000	32.0	32	32	acraneb_transt3\$acraneb3_.LOOP.0037.li.486

COMPUTE

STORE

ANALYZE

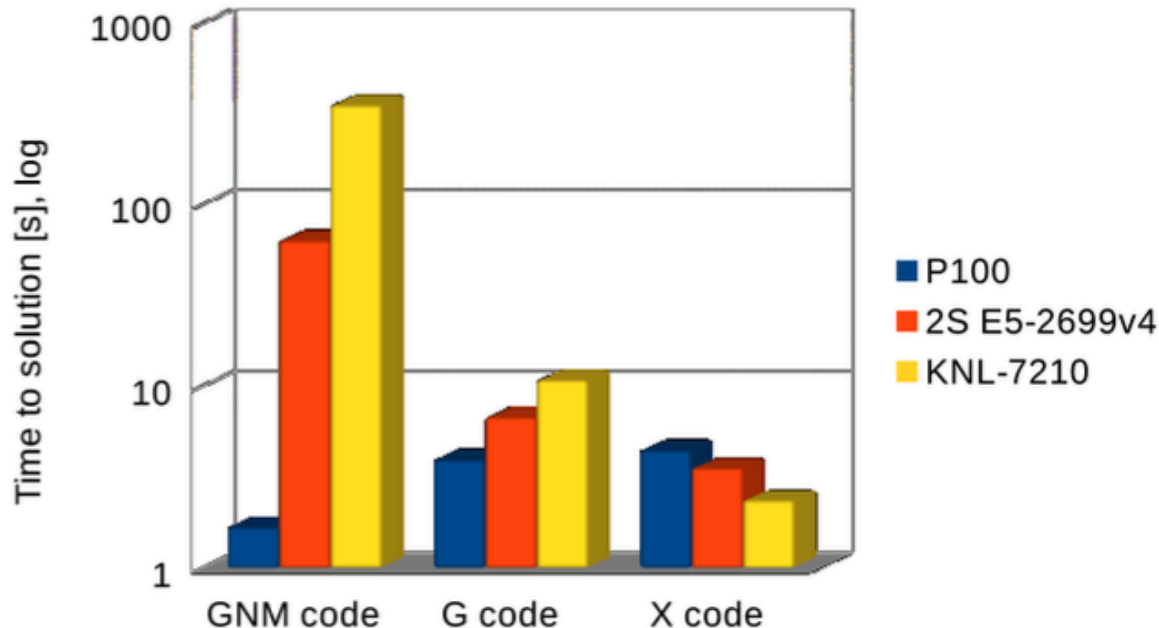
# Tuning for short latency capacity per compute unit



How is the **GN code** performing on the Xeons ?

... Actually, performance drops **A LOT!!!**

- T2S more than **1 min** on BDW and **5 min** on KNL vs **2.3 secs** on P100



# Conclusions



- **The author's of the aforementioned paper and I believe that performance is more important than productivity**
- **For this radiation scheme**
  - The best performance on the GPU does not perform well on KNL and state-of-the-art Xeon
  - The best performance on KNL performs well on Xeon and okay on the GPU.
- **Register spilling to Memory on the GPU hurts performance and rewriting to minimize spills generates code that significantly abuses cache on the Xeon and KNL systems**
- **Perftools is indicating that the principal difference in the two versions of the code is the cache utilization**
- **Memory analysis tool shows that the L2 cache misses on KNL for the G code is ten times what it is for the X code**
- **Memory analysis tool shows that the stalls attributed to memory access are twice as big for the G code on Broadwell than the X code**



---

## **DMI Report 17-22**

### **Tuning the implementation of the radiation scheme ACRANEB2**

Jacob Weismann Poulsen and Per Berg

[http://www.dmi.dk/fileadmin/user\\_upload/Rapporter/TR/2017/SR17-22.pdf](http://www.dmi.dk/fileadmin/user_upload/Rapporter/TR/2017/SR17-22.pdf)